Con2Prim: Recovery of Primitive Variables in Numerical Relativistic Hydrodynamics

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Overview

Outline

- The Einstein Toolkit uses the *Valencia Formulation* of conserved variables for evolving GRMHD.
- In our current work, we only consider fluids without a magnetic field (assume $B^i = 0$).

Equations of State

- 2 main types of EoS:
  1. Analytic:
     - Polytrope: $p(\rho) = \kappa\rho^{\Gamma}, \epsilon(\rho) = \frac{\kappa}{\Gamma-1}\rho^{\Gamma-1}$
     - Ideal Gas (Gamma-Law): $p(\rho, \epsilon) = (\Gamma - 1)\rho\epsilon$
  2. Tabulated:
     - 1 parameter: $p, \epsilon(\rho) = P_p, P_\epsilon(\rho)$
     - 2 parameter: $p, \epsilon(\rho, T) = P_p, P_\epsilon(\rho, T)$
     - 3 parameter: $p, \epsilon(\rho, T, Y_e) = P_p, P_\epsilon(\rho, T, Y_e)$
- Also possible to hybridise analytic and tabulated EoSs e.g.:

$$p(\rho, \epsilon) = P_p^{T=0}(\rho) + (\Gamma_{\mathrm{th}} - 1)\rho\epsilon_{\mathrm{th}}(\rho, \epsilon)$$
$$\epsilon_{\mathrm{th}}(\rho, \epsilon) = \epsilon - P_\epsilon^{T=0}(\rho)$$

N.B. $\epsilon = (\mathcal{E}/m_n) - 1$

The Conserved Variables

- The conserved variables are:
  - D - Density
  - S_i - Momentum
  - τ - Internal energy
- We also use the conserved electron fraction DY_e.
- Evolved variables are multiplied by $\sqrt{\gamma}$.

Expression of Conserved Variables

Conservative Variable	Evolved Quantity	Primitive Expression
D	$\tilde{D} = \sqrt{\gamma} D$	$D = \rho W$
S_i	$\tilde{S}_i = \sqrt{\gamma} S_i$	$S_i = \rho h W^2 v_i$
τ	$\tilde{\tau} = \sqrt{\gamma} \tau$	$\tau = \rho h W^2 - p - D$
DY_e	$\tilde{D} Y_e = \sqrt{\gamma} D Y_e$	$DY_e = \rho W Y_e$

Table of conserved variables, where γ is the determinant of the spacial metric, *rho* is the rest mass density of the fluid, W is the local lorentz factor, h is the specific enthalpy density, v_i is the fluid 3-velocity, p is the (isotropic) fluid pressure, and Y_e is the electron fraction. h, p are calculated from the equation of state of the fluid.

The Problem

- Conserved variables are easily expressed in terms of the primitive variables.
- In general, no analytic expression of the primitive variables in terms of the conserved variables is possible.
- In order to recover the primitive variables, one (or more) of a number of root finding algorithms is used.
- This is a computationally expensive process; in some cases primitive recovery can take $\sim 40\%$ of the total runtime of a simulation.

Motivation

- With the high cost of performing the primitive reconstruction, why not just evolve the conserved variables?
- Two main reasons:
  - The primitive variables are required to construct $T_{\mu\nu}$, used in both the fluid and spacetime evolution
  - v^i is required for the flux terms in the fluid evolution
- We are stuck with having to perform the primitive reconstruction; it is the price we must pay for using the Valencia formulation.

Overview

- Need to use some method of recovering the 6 primitive variables $\boldsymbol{p} = \{\rho, v^i, \{T, \epsilon\}, Y_e\}$ from the 6 conserved variables $\boldsymbol{U} = \{D, S_i, \tau, DY_e\}$.
- It is trivial to obtain Y_e, so the problem is essentially 5 dimensional.
- We will cover 3 different methods for performing this:
  1. 1D Newton-Raphson (NR) in p as in `GRHydro`.
  2. 2D NR in W, T.
  3. Bracketed root finding in hW.

Method Classification

- Methods can be grouped as to whether the solution is bounded or unbounded.
  - NR based methods are unbounded
    - Faster convergence
    - Less stable
  - The bracketed root method is bounded
    - Slower
    - More robust
- Conventional approach:
  1. Try unbounded method
  2. If that fails, use bounded method

1D NR in p

- This is the method shipped with the Einstein Toolkit in `GRHydro`.
- Used mainly for analytic EoSs.
- Quite difficult to use with tabulated EoSs.
- We want to find a root of the equation

$$f(p) = p - \overline{p}\left(\rho\left(\boldsymbol{U}, p\right), \epsilon\left(\boldsymbol{U}, p\right)\right) = 0,$$

where p is the current pressure guess, $\overline{p}(\rho, \epsilon)$ is the EoS of the fluid, and $\rho, \epsilon\left(\boldsymbol{U}, p\right)$ are the density and specific internal energy calculated from p and the conserved variables.

1D NR in p

- The method is based on making iterative guesses for p which are improved upon by using NR on $f(p)$.
- The derivative df/dp is needed:

$$\frac{df}{dp} = 1 - \left.\frac{\partial \rho}{\partial p}\frac{\partial \bar{p}}{\partial \rho}\right|_{\epsilon} - \left.\frac{\partial \epsilon}{\partial p}\frac{\partial \bar{p}}{\partial \epsilon}\right|_{\rho}.$$

- The derivatives w.r.t. p can be calculated analytically from the conserved variables.
- The derivatives of $\bar{p}$ are easily calculated from the EoS if it is analytic, but can become problematic if the EoS is tabular in T.

1D NR in p

- Once the root has been found to the specified precision, the values of ρ, ϵ, p can be used to calculate the remaining primitives.
- If one wishes to use T instead of ϵ as an independant variable in the EoS, an inversion step will be needed to obtain this.
- Performing this inversion step on tabulated EoSs can be a computationally expensive task due to repeated EoS calls.

1D NR in p

- Can also bracket root of $f(p)$ using conserved variables and assumptions of physicality.
- Use bisection to improve the pressure guess.
- Can lead to failure of the T inversion step required for a tabulated EoS, so different methods are needed for a more robust recovery scheme.

2D NR in W, T

- For EoSs based on T, it makes sense to use a scheme that solves for this directly.
- This removes the need for an expensive T inversion stage $\Rightarrow$ make recovery method faster and more robust.
- Currently working on the implementation of a 2D NR method derived in [Siegel et al., 2018], based on work by [Antón et al., 2006].

2D NR in W, T

- The roots to be solved in this method are

$$f_1(W, T, \boldsymbol{U}) = [\tau + D - z + p]\, W^2,$$
$$f_2(W, T, \boldsymbol{U}) = \left[z^2 - S^2\right] W^2 - z^2,$$

  where $z = \rho h W^2$ and p are calculated throught the EoS using $\rho = D/W$ and $Y_e = DY_e/D$.

- In order to perform NR, we need the Jacobian of this system.

2D NR in W, T

- The four derivatives required to write down the Jacobain are:

$$\frac{\partial f_1}{\partial W} = 2W\left[\tau + D - z + p\right] + W^2\left[\frac{\partial p}{\partial W} - \frac{\partial z}{\partial W}\right]$$

$$\frac{\partial f_1}{\partial T} = W^2\left[\frac{\partial p}{\partial T} - \frac{\partial z}{\partial T}\right]$$

$$\frac{\partial f_2}{\partial W} = 2W\left[z^2 - S^2\right] + 2z\left[W^2 - 1\right]\frac{\partial z}{\partial W}$$

$$\frac{\partial f_2}{\partial T} = 2z\left[W^2 - 1\right]\frac{\partial z}{\partial T}$$

2D NR in W, T

- The derivatives of z and the derivatives w.r.t. W can be written in terms of EoS derivatives:

$$\frac{\partial p}{\partial W} = -\frac{D}{W^2}\frac{\partial p}{\partial \rho}$$

$$\frac{\partial z}{\partial W} = D\left[1 + \epsilon - \frac{D}{W}\frac{\partial \epsilon}{\partial \rho}\right] + 2pW - D\frac{\partial p}{\partial \rho}$$

$$\frac{\partial z}{\partial T} = DW\frac{\partial \epsilon}{\partial T} + W^2\frac{\partial p}{\partial T}$$

- These derivatives are more stable for an EoS table given in terms of ρ, T, Y_e than those in the first method.

2D NR in W, T

- This method is both faster and better behaved than the previous method for a tabulated EoS.
- NR convergence may still stall or fail; we want a backup method should this happen.
- Insted of the pressure based bisection method mentioned previously, we choose a variation of another method presented in [Siegel et al., 2018] that brackets hW.

Bracketed Root Finding

- Instead of using an unbounded method such as NR, some methods find a root in a quantity that is known to be between two values.
- By doing this we can avoid derivatives of the EoS, greatly improving stability for tabulated EoSs.
- We will cover one such method that solves for the value of hW.

Bracketed Root Finding in hW

- We will be solving the root of the equation

$$f(x) = x - \hat{h}\hat{W}$$

  where $x = hW$ is our unknown, and $\hat{}$ denotes that the quantity is calculated using $\boldsymbol{U}$, the EoS, and the current guess for x.
- It can be shown that the root of $f(x)$ will satisfy the condition

$$1 + \frac{\tau}{D} \leq x \leq 2\left(1 + \frac{\tau}{D}\right).$$

- We can then use any of a number of bracketed root finding methods such as bisection, Dekker's method, Brent's method, etc.

Bracketed Root Finding in hW

- $\hat{h}$, $\hat{W}$ are calculated throught the following:

$$\hat{W}^{-2} = 1 - \frac{S^2}{x^2 D^2},$$
$$\hat{\epsilon} = -1 + \frac{x}{\hat{W}}\left[1 - \hat{W}^2\right] + \hat{W}\left[1 + \frac{\tau}{D}\right].$$

- The EoS is then inverted to find $\hat{T}$ given $\hat{\rho} = D/\hat{W}$, $\hat{\epsilon}$, and $Y_e = DY_e/D$.
- The EoS is then used to find $\hat{p}$ using $\hat{\rho}$, $\hat{T}$, and Y_e.
- Finally, $\hat{h}$ is given by $\hat{h} = 1 + \hat{\epsilon} + \hat{p}/\hat{\rho}$.

Bracketed Root Finding in hW

- There are, however, some caveats that should be mentioned:
  - This method (as with any method that does not solve for T directly) requires a T inversion step for tabulated EoSs.
  - It is also possible that a given x does not correspond to a physical region of the EoS (i.e. for a given x, T inversion may be impossible).
- While the first of these means out root finding will be slow, the second can be fatal to the method.
- It is this second issue that our extended method is designed to circumvent.

Bracketed Root Finding in hW

- If one of the initial guesses for the bracket of x is unphysical, the method cannot proceed, so we propose the following extension, should this be the case.
- Assume $f(x)$ was calculated successfully at the bottom end of the bracket (if it was the other root that was successful, the directions in the method are swapped).
- We begin by defining the following:
  - x_{max} is the lowest position where the root failed
  - x_{min} is the highest position where the root takes the same sign as the successful root
- For the first iteration, $x_{min} = 1 + \tau/D$ and $x_{max} = 2 + 2\tau/D$.

Bracketed Root Finding in hW

- To obtain a bracket on x, we iterate the following procedure:
  1. Calculate $x_{temp} = (x_{max} + x_{min})/2$
  2. Calculate $f(x_{temp})$
     - If $f(x_{temp})$ could not be calculated, we set $x_{max} = x_{temp}$ and loop.
     - If $f(x_{min}) \times f(x_{temp}) \leq 0$ then we can use these values as our bracket and proceed with the root finding.
     - If If $f(x_{min}) \times f(x_{temp}) > 0$ then we set $x_{min} = x_{temp}$ and loop.
- This method can also be extended to the case that neither of the initial values could be used successfully by performing a brute force search in the initial bracket, then attempting to find a bracket using the above method on either side of the found value.

Overview

- Performing primitive recovery is a necessary consequence of using the Valencia formulation.
- In the General Relativisitic Hydrodynamics case, it is essentially a 5D problem.
- It can be a computationally expensive part of a simulation.
- Different methods are more suited to different types of EoS.

Method comparison

- We have studied 3 different methods for performing primitive recovery, with the following pros and cons:

Method	Pros	Cons
1D NR in p	Good for analytic EoSs Easy to bracket if NR fails	Poor derivatives for tabulated EoSs T inversion required for tabulated EoSs
2D NR in W, T	Derivatives are along table axes T is solved for directly	No bracket if NR fails
Bracketed in hW	Bracketed methods guarantee convergence No derivatives needed	T inversion required for tabulated EoSs Can be very slow if brackets must be modified

Comparison of pros and cons for different primitive recovery schemes.

- As with [Siegel et al., 2018], we propose a combinantion of methods be used to perform primitive recovery, namely 2D NR in W, T with bracketed root finding in hW as a fallback.

References

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